Contradiction of the DENSITY MATRIX notion in quantum mechanics

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Abstract

It is shown that description of a nonpolarized neutron beam by density matrix is contradictory. Density matrix is invariant with respect to choice of quantization axis, while experimental devices can discriminate between different quantization axes.

> —*The statement in the title is evidently wrong at the modern level of knowledge. The density matrix is not an auxiliary construction but a result of basic concepts of quantum mechanics. More over experience with this notion is huge and convincing. As for the given paper, no doubt it contains an error. It is in inexactitude of wordings and reasonings. The problem is only how to find this error. However it is a task for the author.*
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> Referee of JETP Lett.

1   Introduction

The main notions in nonrelativistic quantum mechanics are the Schrödinger equation and wave function $|\psi\rangle$. The density matrix is an artificial construction, which, as will be shown bellow, can be contradictory. We will consider the simplest case of the density matrix, describing a monochromatic nonpolarized neutron beam.

A monochromatic non polarized neutron beam is characterized by the density matrix

$$\rho = \frac{1}{2}\Big(|u\rangle\langle u| + |d\rangle\langle d|\Big), \tag{1}$$

which is one half of the unit matrix. The states $|u, d\rangle$ correspond to wave functions for neutrons polarized along and opposite some direction, which is known as quantization axis. The choice of the quantization axis, however, is not important, because the density matrix Eq. (1) is invariant with respect

to such a choice. Indeed, if one chooses the quantization axis along some unit vector $\boldsymbol{a}$, then the matrix Eq. (1) becomes

$$\rho = \frac{1}{2}\Big(|\boldsymbol{a}\rangle\langle\boldsymbol{a}| + |-\boldsymbol{a}\rangle\langle-\boldsymbol{a}|\Big). \tag{2}$$

If one chooses another axis $\boldsymbol{b}$, then, since

$$|\boldsymbol{a}\rangle = \alpha|\boldsymbol{b}\rangle + \beta|-\boldsymbol{b}\rangle, \qquad |-\boldsymbol{a}\rangle = \alpha^*|-\boldsymbol{b}\rangle - \beta^*|\boldsymbol{b}\rangle, \tag{3}$$

where $|\alpha|^2 + |\beta|^2 = 1$, one obtains

$$\rho = \frac{1}{2}\Big([\alpha|\boldsymbol{b}\rangle + \beta|-\boldsymbol{b}\rangle]\,[\alpha^*\langle\boldsymbol{b}| + \beta^*\langle-\boldsymbol{b}|] +$$

$$+ [\beta^*|\boldsymbol{b}\rangle - \alpha^*|-\boldsymbol{b}\rangle]\,[\beta\langle\boldsymbol{b}| - \alpha\langle-\boldsymbol{b}|]\Big) =$$

$$= \frac{1}{2}\Big(|\boldsymbol{b}\rangle\langle\boldsymbol{b}| + |-\boldsymbol{b}\rangle\langle-\boldsymbol{b}|\Big). \tag{4}$$

For instance, if $\boldsymbol{a}$ is along y axis, and $\boldsymbol{b}$ is along z-axis, one has

$$|y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}}\left(|z\rangle + i|-z\rangle\right), \qquad |-y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left[|-z\rangle + i|z\rangle\right], \tag{5}$$

and

$$\rho = \frac{1}{2}\Big(|+z\rangle\langle+z| + |-z\rangle\langle-z|\Big) = \frac{1}{2}\Big(|+y\rangle\langle+y| + |-y\rangle\langle-y|\Big). \tag{6}$$

So two axes are equivalent for the density matrix. However these axes can be discriminated by an experimental equipment, and our goal is to show how it is possible. To achieve it let's first show how one can find polarization direction of a polarized beam.

2 A method for polarization direction measurement

The principle is based on an effect known in neutron optics [1–3], and is related to spin flip with the help of a resonant radio frequency (rf) spin-flipper. Such a spin-flipper is a coil with a permanent magnetic field $\boldsymbol{B}_0$ and perpendicular to it rotating counterclockwise rf-field

$$\boldsymbol{B}_{rf} = b\Big(\cos(\omega t), \sin(\omega t).0\Big), \tag{7}$$

where $\omega = 2\mu B_0/\hbar$, and μ is magnetic moment of the neutron, which is aligned oppositely to the neutron spin $\boldsymbol{s}$. Direction of $\boldsymbol{B}_0$ can be accepted as the quantization z-axis. Interaction of neutrons with such a flipper can be solved exactly and analytically, and the solution can be explained as follows [3].

The neutron interaction with magnetic field is described by the potential $-\boldsymbol{\mu}\cdot\boldsymbol{B}_0$. Therefore neutrons in the state $|z\rangle$ entering the field $\boldsymbol{B}_0$ are decelerated because the field in this case creates a potential barrier of height μB_0.

Inside the flipper the rf-field turns the spin down, i.e. transforms the state $|z\rangle$ into $|-z\rangle$. In this state the interaction $-\boldsymbol{\mu}\cdot\boldsymbol{B}_0$ becomes negative, so the potential barrier transforms into potential well of depth μB_0. Therefore after exit from the flipper and its magnetic field $\boldsymbol{B}_0$ the neutron decelerates once again. In total the neutron energy after transmission through the spin flipper decreases by amount $2\mu B_0$, which means emission of an rf quantum: $\hbar\omega = 2\mu B_0$. The wave functions before and after spin flipper are

$$|\psi_{in}(x,t)\rangle = \exp(ikx - i\Omega t)|z\rangle, \tag{8}$$

$$|\psi_{out}(x,t)\rangle = \exp(ik_-(x-D) - i(\Omega - \omega)t)|-z\rangle, \tag{9}$$

respectively. Here x is the axis of propagation, D is thickness of the spin-flipper, k is initial wave number, $\Omega = \hbar k^2/2m$, m is the neutron mass, and $k_- = \sqrt{k^2 - 2m\omega/\hbar}$. If the incident neutron has the state $|-z\rangle$ it accelerates, and after spin-flipper has energy larger than original one by the amount $2\mu B_0$, which means absorbtion of an rf quantum: $\hbar\omega = 2\mu B_0$. The wave functions before and after spin flipper in this case are respectively

$$|\psi_{in}(x,t)\rangle = \exp(ikx - i\Omega t)|-z\rangle, \tag{10}$$

$$|\psi_{out}(x,t)\rangle = \exp(ik_+(x-D) - i(\Omega + \omega)t)|z\rangle, \tag{11}$$

where $k_+ = \sqrt{k^2 + 2m\omega/\hbar}$.

If the incident neutron has a polarization $|\xi\rangle = \alpha|z\rangle + \beta|-z\rangle$, its wave function before and after spin flipper are respectively

$$|\psi_{in}(x,t)\rangle = \exp(ikx - i\Omega t)(\alpha|z\rangle + \beta|-z\rangle), \tag{12}$$

$$|\psi_{out}(x,t)\rangle = \alpha\exp(ik_-(x-D) - i(\Omega - \omega)t)|-z\rangle +$$
$$+ \beta\exp(ik_+(x-D) - i(\Omega + \omega)t)|z\rangle. \tag{13}$$

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The spin arrow of this state represents a rotating spin wave propagating along x-axis.

Let's put at some position $x = x_0$ an analyzer, which transmits only neutrons polarized along y-axis. Since

$$|+z\rangle = \frac{1}{\sqrt{2}}(|+y\rangle - i|-y\rangle), \qquad |-z\rangle = \frac{1}{i\sqrt{2}}(|+y\rangle + i|-y\rangle), \quad (14)$$

where $|\pm y\rangle$ denote states with polarization along and opposite y axis, the neutron state Eq. (13) after the analyzer is

$$|\psi_{+y}(x_0, t)\rangle =$$

$$\frac{|+y\rangle}{i\sqrt{2}} \left(\alpha e^{ik_-(x_0-D)-i(\Omega-\omega)t} + i\beta e^{ik_+(x_0-D)-i(\Omega+\omega)t} \right), \quad (15)$$

and intensity of the neutron beam after the analyzer at some position x_0 is

$$I_{+y}(x_0, t) = \frac{1}{2} \left[|\alpha|^2 + |\beta|^2 + 2|\alpha\beta| \cos(\varphi + 2\omega t) \right], \quad (16)$$

where φ is some phase. We see that the beam has density modulation with time, and visibility of the modulation

$$V = \frac{2|\alpha\beta|}{|\alpha|^2 + |\beta|^2} = \frac{2|\alpha/\beta|}{1 + |\alpha|^2/|\beta|^2} \quad (17)$$

determines ratio $|\alpha/\beta|$ and, therefore, the polar angle of the incident neutron spin arrow with respect to z-axis. If α or β are zero, i.e. incident neutron is polarized along or opposite spin-flipper axis, oscillations are absent.

3 An experimental possibility for discrimination between z and y quantization axes

Now let's suppose that quantization axis is directed along y-axis. It means that the number N_+ of particles in the state $|+y\rangle$ is the same as the number N_- in the state $|-y\rangle$. Since $|\pm y\rangle = (|\pm z\rangle + i|\mp z\rangle)/\sqrt{2}$, we have according to Eq. (15) the intensities after y-analyzer for two incident components $|\pm y\rangle$ measured by a detector at some position x_0 to be

$$I_{+y}^{\pm}(x_0, t) = \frac{N_\pm}{2} \left[1 \pm \cos(2\omega t) \right], \quad (18)$$

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where upper index points out what was the incident component, and for simplicity we put the phase φ in Eq. (18) to zero, because it is the same for all the particles.

The sum of averaged over time two intensities is a constant

$$\langle I_{+y}(t)\rangle = \langle I_{+y}^{+}(t)\rangle + \langle I_{+y}^{-}(t)\rangle =$$

$$= \frac{\langle N_{+}\rangle}{2}\left[1 + \cos(2\omega t)\right] + \frac{\langle N_{-}\rangle}{2}\left[1 - \cos(2\omega t)\right] = N_0, \tag{19}$$

where $N_0 = \langle N_{+}\rangle = \langle N_{-}\rangle$.

However besides the average value there are also fluctuations of neutron count rate. We can naturally suppose that the fluctuations of two incident spin components are independent, and obey the Poisson statistics. Then fluctuations of neutron flux density after y-analyzer will be

$$\langle |\delta I_{+y}(t)|^2\rangle = \langle |\delta I_{+y}^{+}(t)|^2\rangle + \langle |\delta I_{+y}^{-}(t)|^2\rangle =$$

$$= \left\langle \frac{\delta N_{+}}{2}\left[1 + \cos(2\omega t)\right]\right\rangle^2 + \left\langle \frac{\delta N_{-}}{2}\left[1 - \cos(2\omega t)\right]\right\rangle^2 = \frac{N_0}{2}(1 + \cos^2(2\omega t)). \tag{20}$$

To see these oscillations one should divide the period $T = \pi/2\omega$ over N small intervals $\Delta T = T/N$ and sum the value

$$\frac{\langle |\delta I_{+y}(t_n)|^2\rangle}{N_0} = \frac{1}{2}\left[1 + \cos^2(t_n/T)\right], \tag{21}$$

at $t_n = n\Delta T$ over many periods T.

This way one can discriminate between two quantization axes z, and y. Therefore these quantization axes are not equivalent, whereas according to density matrix expression they are absolutely equivalent. This is the contradiction we wanted to point to.

4 Conclusion

The main element of quantum mechanics is a wave function, and corresponding to it a pure state. If one has an ensemble of particles with different pure states, and the distribution of different states is characterized by probabilities, one must calculate a process with pure states and then average over probabilities. This is the way neutron scattering cross sections are calculated. First they

are calculated for a pure state of an incident plain wave, and then the obtained cross section is averaged over probability distribution of the incident plain waves. Of course the density matrix also can be useful, but because of discovered contradiction, one must be very careful with it.

Список литературы

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